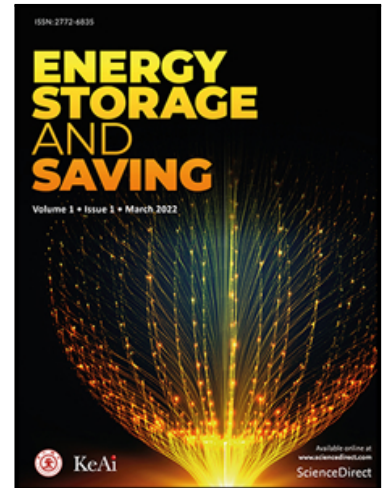


Journal Pre-proof

Thermal Energy Storage as a Way to Improve Transcritical CO₂ Heat Pump Performance by Means of Heat Recovery Cycles

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HIGHLIGHTS

- A combination of a water tank as heat storage and a transcritical CO₂ heat pump with two different evaporators can increase COP by means of heat recovery cycles.
- A percentage raise of 4.43% on the base cycle's COP has been verified through dynamic modelling of the system.
- Tank volume mainly affects charging and discharging time

Journal Pre-proof

Thermal Energy Storage as a Way to Improve Transcritical CO₂ Heat Pump Performance by Means of Heat Recovery Cycles

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Abstract

Electrification of the heating sector is a major target of energy transition towards a more sustainable, efficient, and less polluted future. Heat pumps are considered more suitable than electrical heaters or fossil-fueled boilers; however, common refrigerants cause ozone layer depletion, which exacerbates the greenhouse effect. Natural refrigerants, such as CO₂, perform comparably and even better than hydrofluorocarbons while minimizing the negative aspects. This study presents a model of a water-heater CO₂ transcritical heat pump in a configuration that increases the overall coefficient of performance (COP) by introducing thermal energy storage (TES). The thermodynamic cycle was divided into two separate phases. After heating the TES (charging), warm water was used as the heating fluid in the evaporator to increase the evaporation temperature and pressure of CO₂, which reduced the work of the compressor. As the water temperature decreased progressively, the discharge cycles improved the total COP. The case study focuses on dairy processes and suggests a more straightforward and cheaper method to improve cycle efficiency than the current processes, such as ejector-expansion systems or double compression.

Keywords

Energy efficiency, Natural refrigerants, CO₂ heat pump, Thermal energy storage, Dairy industry

[1] Introduction

Along with ammonia and sulfur dioxide, carbon dioxide was used as a refrigerant during the first decades of the previous century, until freons were introduced as better, safer, and less environmentally harmful alternatives. However, the scenario changed completely after the

identification of direct and indirect toxic effects that ranged from suffocation or injuries due to dissociation products to more significant issues such as ozone depletion and greenhouse effects [1].

The Montréal Protocol of 1987 [2] marked the history of the refrigeration, air-conditioning, and heating sectors by progressively banning chlorofluorocarbons and hydrochlorofluorocarbons, and promoting alternatives with lower ozone depleting potential (ODP) and minimum global warming potential (GWP), such as CO₂. The so-called “renaissance” of carbon dioxide as a refrigerant which began in the mid-1990s can be attributed to Gustav Lorentzen, a pioneer in using CO₂ in refrigeration or heat pump cycles [3]. He built and tested one of the first prototypes, namely an automotive air conditioning system which showed promising results [4]. Carbon dioxide can be found everywhere, is nontoxic and inflammable, and possesses peculiar thermodynamic and thermophysical properties that make it suitable as a refrigerant in vapor compression systems. Because of its relatively low critical pressure (approximately 73 bar, 31 °C), CO₂ is primarily used in transcritical thermodynamic cycles where heat rejection occurs significantly above the critical temperature. In this region, pressure and temperature are mutually independent. Therefore, the process is performed by a gas cooler and not by a condenser, and the pressure remains constant while the temperature varies within a rather wide range. Because of the smooth temperature difference between the fluids, this temperature profile makes CO₂ ideal whenever a large increase in temperature is required. This includes processes such as sanitary hot water production or heat transfer to processes at different temperature levels by combining loads [5].

Electrification of the heating sector can easily be achieved by using heat pumps instead of classic boilers or electric heaters [6]. Transcritical CO₂ heat pumps can operate in a wide range of heat rejection pressures and evaporation conditions, and the typical coefficient of performance (COP) values primarily varies according to the required heat loads. According to Artuso et al. [7], the average COPs for an air-to-water R744 heat pump model that provides district hot water and space heating range between 3–3.50 (considering maximum pressure and evaporating temperatures of 105 bar and approximately 0 °C, respectively). An experimental water-to-water system built to simulate the Harbin cold conditions exhibits COP fluctuations between 2.14–2.40 at a constant evaporating temperature of 8 °C and various high pressures [8]. The use of ejectors and multi-ejector systems for expansion work recovery remains an ongoing research subject; however, positive relative COP differences of up to 8% with respect to valve expansion have been demonstrated [9].

In terms of civil and residential applications, several authors have discussed CO₂ heat pumps with regard to civil and residential applications. Water heaters were modeled by Nekså [10] and White et al. [11], and comparisons between experimental systems that utilized CO₂ and R134a confirmed that transcritical cycles achieve higher COPs when a significant temperature increase is required [12], such as in sanitary hot water demand. Space and water heating for civil and residential needs have been thoroughly discussed and several CO₂ transcritical heat pumps are already commercially available. These include the EcoCute model produced by six Japanese manufacturers (Denso, Daikin, Sanyo, Matsushita Electric Industrial, Hitachi Appliances, Mitsubishi Electric, and Sanden) and marketed under approximately 14 names.

Industrial processes account for 51% of the energy consumed for heating and are covered by fossil fuel equipment [13]. Nevertheless, industrial applications of heat pumps are still being studied. Although hydrofluorocarbon (HFC) heat pumps are suitable for fields with a steady demand for heat at medium temperatures and waste heat to be reused, as described in the early 1980s by the NEI Project [14], transcritical CO₂ heat pumps can achieve higher heat rejection temperatures than HFCs. This makes them attractive in the food processing industry for processes such as sterilization, pasteurization, blanching, evaporation, drying [15], food canning, and brewing, or at dairy facilities. Singh and Dasgupta [16] proposed a basic system

for waste heat recovery coupled with ammonia-based refrigeration to preheat boiler water for pasteurization and cleaning in place (CIP).

A new layout of a transcritical CO₂ heat pump for a dairy process, which was studied and modeled by Liu et al. [17], resulted in primary energy savings of approximately 36.0% and 45.1% for the milk and cheese processes, respectively, compared to those of fossil-fueled boilers. Energy savings compared to those of ammonia heat pumps in the simultaneous cooling and heating in the food processing industry strongly depend on the loads and technical specifications [18].

Technical improvements are crucial for enhancing the overall performance of these systems and simple solutions, such as regenerative heat exchangers, known as internal heat exchangers (IHX), are now standard. Robinson et al. [19] obtained a 7% increase in the COP when an IHX was added to a basic transcritical CO₂ heat pump system. However, other researchers are still investigating the benefits of an ejector expansion system. For example, Dasi et al. [20] built a model validated by an experimental test setup and confirmed the utility of the IHX and its potential use in milk pasteurization.

However, these solutions are neither cheap nor easy to realize and manage, and are often commercially unviable. Therefore, in this study, we propose an easy and original solution for improving the COP of a CO₂ heat pump, which uses the TES along with a reversible heat pump capable of switching its heat source from air to warm water when necessary.

2. Method

Figure 1 shows a schematic of the heat pump and hydronic circuit, which compete to increase efficiency.

Similar to parallel compression, this solution facilitates energy recovery without requiring a second compressor when the outlet temperature at the gas cooler remains high, which often occurs when the heat demand from the heating system is limited.

To explain the function of the system, we refer to two distinct heat transfer stages.

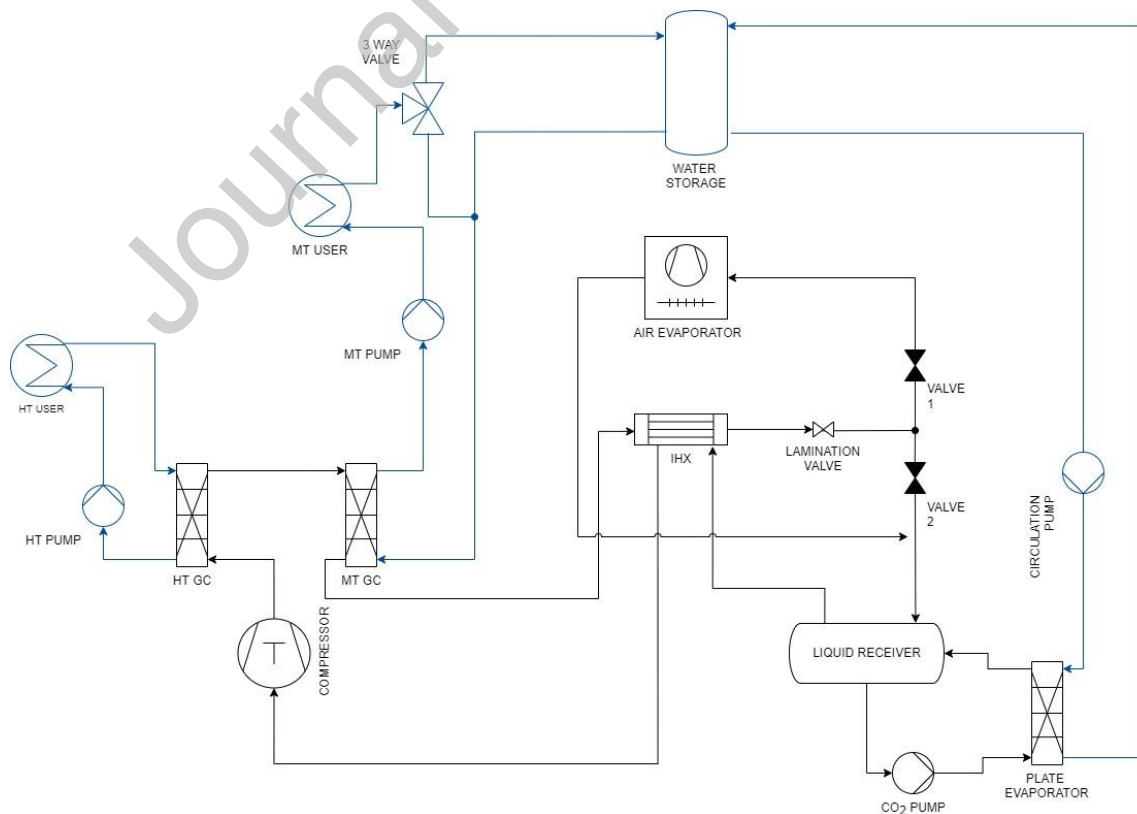


Fig. 1. Schematic of the heat pump and hydronic layout. High temperature (HT); medium temperature (MT); gas cooler (GC); internal heat exchangers (IHX).

2.1 Charging phase

High-pressure and high-temperature CO₂ discharged from the compressor rejected heat to the water by first passing through a High-temperature gas cooler (HT GC) and then through a medium-temperature gas Cooler (MT GC). Hot water directly served high-temperature users (HT USER), whereas warm water was first supplied to medium-temperature users (MT USER) and then used to warm the water in the storage. The refrigerant was further cooled in the IHX, whereas the CO₂ on the other side was at the pressure and temperature of the receiver. A lamination valve performed isenthalpic expansion until the saturation pressure (that depends on the ambient temperature) was reached. CO₂ absorbed heat through the AIR EVAPORATOR by passing through VALVE 1 (while VALVE 2 was closed). The liquid refrigerant was collected in the receiver and drawn for superheating in the IHX before being compressed again.

2.2 Discharging phase

The refrigerant followed the same path to the lamination. However, it was directly sent to the liquid receiver through VALVE 2 (while VALVE 1 was closed). Liquid CO₂ from the receiver was pumped into a plate heat exchanger to be heated by warm water from the TES, whereas saturated CO₂ vapor was heated through the IHX and then compressed. Considering the hydronic circuit, the requirements of the HT and MT users were still met, but water was removed from the tank and continuously recirculated (i.e., the discharging phase).

The pressure-enthalpy diagrams in Figs. 2 and 3 show the thermodynamic cycles of the two phases. Compression from P1 to P2 takes carbon dioxide to a supercritical state above the saturation curve, such that readily transfers its energy content to end users through an isobaric heat rejection from P2 to P3 that occurs in the two gas coolers described previously. During the charging phase (Fig. 2), low-quality heat warms up water in the TES and the residual heat is used in the regeneration process in the IHX to ensure superheated conditions gas at the inlet of the compressor (processes P3–P4 and P6–P1). After the valve expansion (P4–P5), CO₂ finally evaporates in an ambient air heat exchanger (P5–P6).

Therefore, thermal energy was produced as in a conventional transcritical cycle and the low-temperature heat still available in the gas cooler was temporarily collected and stored as sensible heat in the tank. This process is essentially free because the additional heat removed from the cold source by cycle extension is stored at a higher temperature without additional compression costs. This phase continued until the entire stratified tank attained this temperature.

During the discharge phase, a water evaporator was fed directly from the stratified storage. As evaporation occurs in saturation conditions, the temperature and pressure are mutually dependent. When warm water is sent, the evaporation pressure is higher, and the compressor performs less work (P1–P6 in Fig. 3). The water temperature and evaporation pressure progressively decrease, leading to a series of heat recovery cycles that improve the total COP. Therefore, in the discharging phase, a cycle with a higher and progressively decreasing evaporation temperature is used until the thermal storage is fully consumed, as shown in Fig. 4 in which the recovery phase has been discretized into six subcycles. The discharging phase starts with the highest possible evaporation temperature which corresponds to the lowest compressor work (yellow cycle in Fig. 4). As the TES discharges heat, its temperature, as well as the evaporation temperature during the discharging cycles progressively decrease, as shown in Fig. 4. The system returns to its charging mode when the TES is completely discharged.

2.3 Dynamic model of the transcritical CO₂ heat pump

The dynamic model of the transcritical carbon dioxide heat pump was built on the Dymola platform [21]. This is a powerful multidomain system based on the object-oriented language Modelica [22] and augmented by the TIL Suite [23], an external software with professional libraries for modeling thermodynamic systems and their interactions.

Two separate models were considered for the charging and discharging phases, as shown in Figs. 5 and 6. They share the same components because they represent the same heat pump in two different periods. The compressor was modeled using the *effCompressor* model, which was modified to suit the semi-hermetic CD6 801-53M compressor from Dorin Innovation [24] by adding tables to calculate the isentropic and volumetric efficiencies. The gas coolers and plate evaporator in the discharging model were modeled as plate heat exchangers using the *VLEFluidLiquid ParallelFlowHX* module. The air evaporator and IHX were modeled as a fin-and-tube heat exchanger (*MoistAirVLEFluid ParallelFlowHX*) and plate heat exchanger (*VLEFluidVLEFluid ParallelFlowHX*), respectively. Both schemes had lamination and bypass valves for controlling the suction temperature when the IHX was insufficient.

Thermal energy storage was modeled as a closed and pressurized water tank, whose charge was regulated by a three-way valve that switched its position from feeding to bypassing the tank when a temperature of 30 °C was reached.

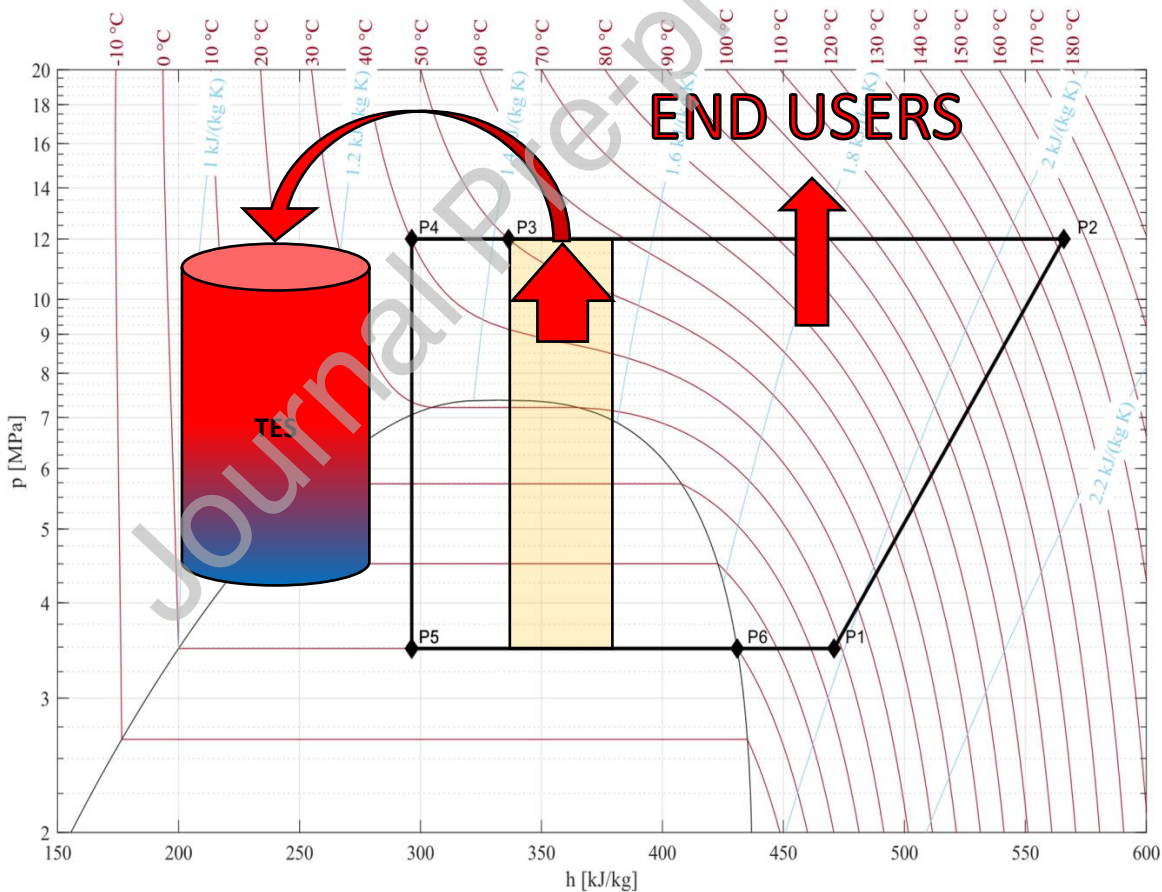


Fig. 2. Pressure-enthalpy diagram of the charging phase. Thermal energy storage (TES).

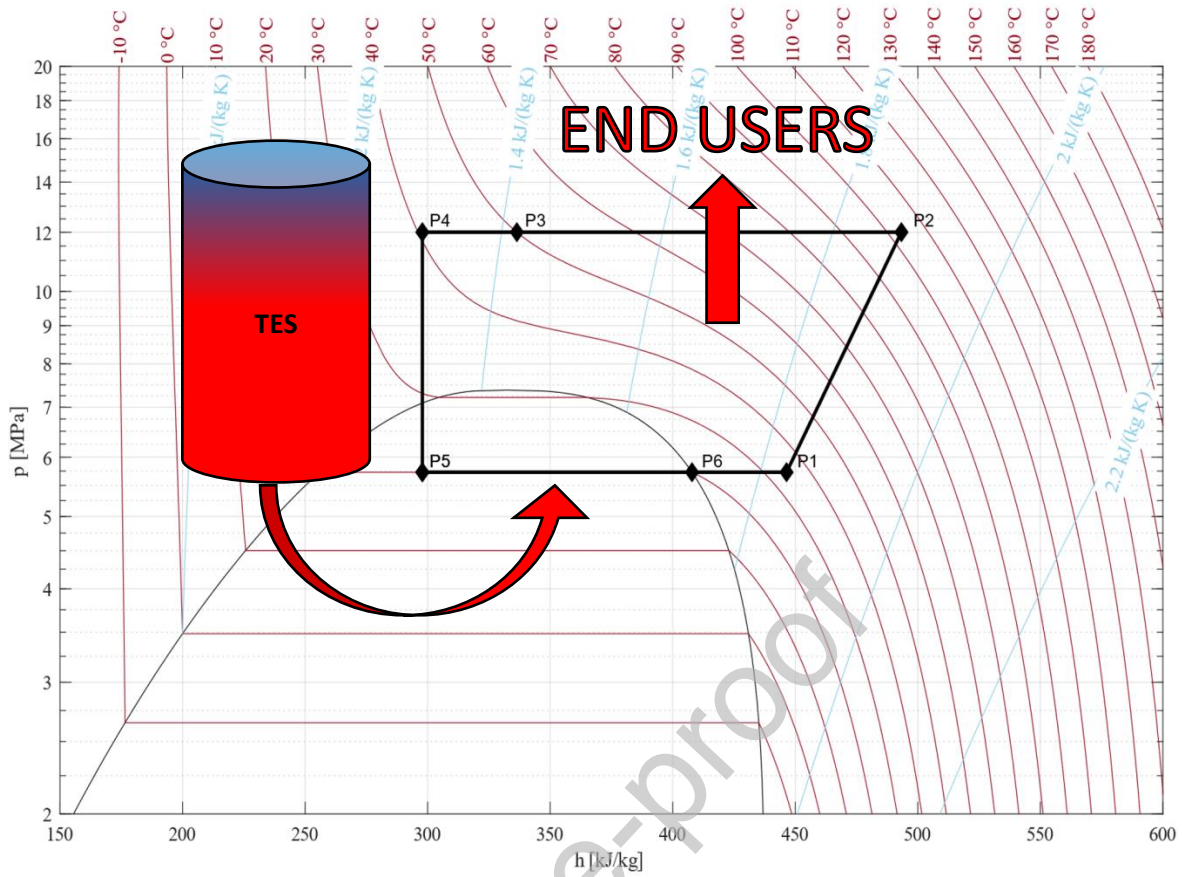


Fig. 3. Thermodynamic cycle of the discharging phase in the pressure-enthalpy diagram

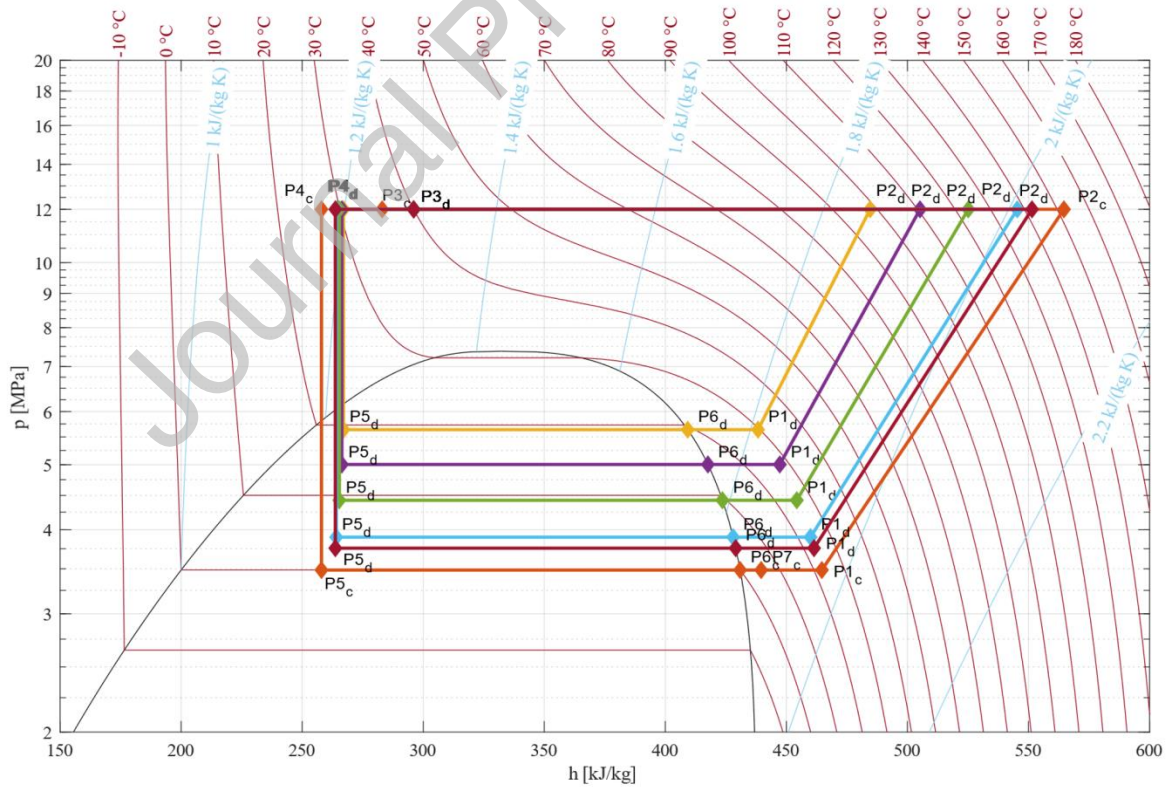


Fig. 4. Thermodynamic cycles of the discretized heat recovery phases in the pressure-enthalpy diagram

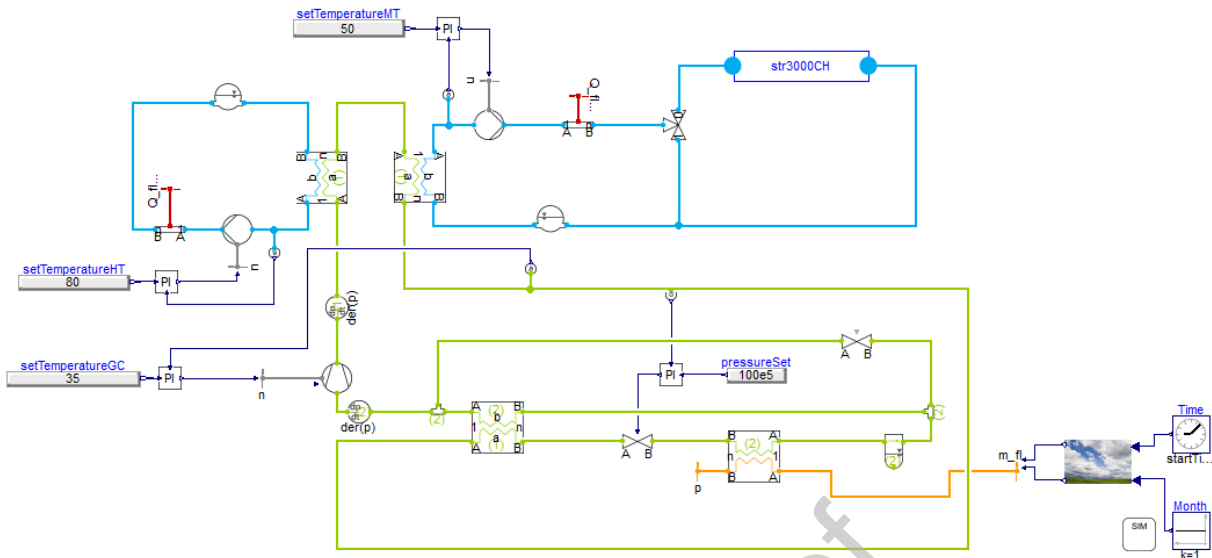


Fig. 5. Dynamic model of the charging phase

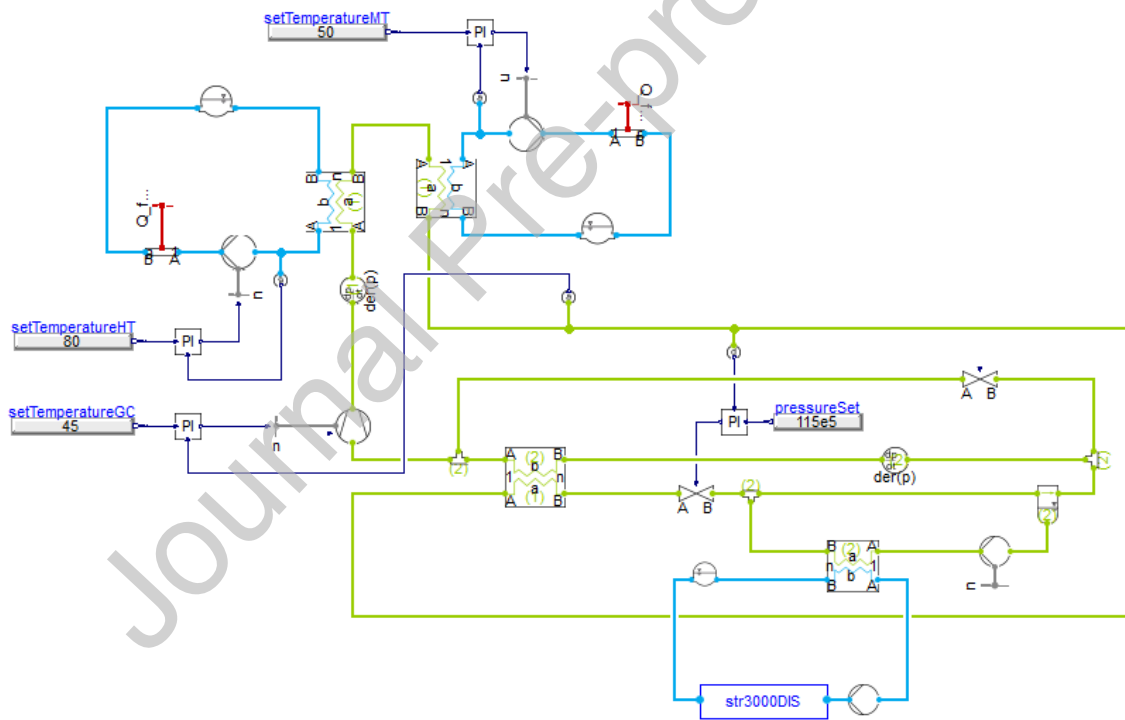


Fig. 6. Dynamic model of the discharging phase

Two proportional-integral controls were implemented and tuned to achieve and maintain the desired water temperature by controlling the water mass flow rate of the pump. On the CO₂ side, the temperature outside the MT gas cooler was maintained by varying the compressor speed, while the maximum pressure was regulated by opening the expansion valve.

In the charging model, the boundary conditions were the ambient temperature and relative humidity of a typical day for every month of the solar year at a typical location in central Italy. The users were the same for both the charging and discharging schemes and are simply

considered as *heatBoundaries* where hot and warm water flow and cool down while a certain amount of heat is extracted.

Pressure losses in the gas coolers and IHX were calculated with a quadratic dependence on the mass flow rate using the conditions at a nominal point known from the designer datasheets.

The nominal total heating capacity was 190 kW, while HT, MT, air temperature, and evaporation temperature were (60–80 °C), (15–70 °C), –5 °C, and –11 °C, respectively. The components were modeled on real components and their design characteristics are listed in Table 1.

Heat losses to the environment from the compressor and other components were neglected.

Table 1. Design characteristics of the most relevant components.

Component	Model	Design characteristics
Compressor	DORIN CD6 801-53M	Displacement 6.1163e-4 m ³ , variable speed
Gas cooler HT	SWEP B185Hx80/1P	Plate heat exchanger, heat transfer area 5.90 m ²
Gas cooler MT	SWEP B185Hx125/2P	Plate heat exchanger, heat transfer area 9.31 m ²
Internal Heat Exchanger	-	Plate heat exchanger, heat transfer area 4.23 m ²
Liquid receiver	Enex	Pressure 80 bar, total volume 260 l
Lamination valve	-	Effective flow area 6.882e-6 m ²
Water evaporator	Alfa Laval	Brazed plate heat exchanger, heat transfer area 17.70 m ²
Air evaporator		Fin-and-tube heat exchanger
Water pumps	Grundfos TP 32-120/2 A-F-A-BOQE-DX1	Single-stage, closed centrifugal
CO ₂ liquid pump	Hy-save 833-SS-080-VSD-B-K65	Centrifugal

2.4 Case Study

The heat demand of dairy plants accounts for a major part of the total energy consumed. Approximately 80% of this energy is used for heating and cleaning using hot water or steam produced by the combustion of fossil fuels [25]. Regardless of the final product, heat is used in almost all processes including those for processing milk, butter, and cheese. This study considers pasteurization and yoghurt fermentation as HT and MT users, respectively, because of the matching heat-rejection profile temperatures. During pasteurization, raw milk is exposed to a high temperature for a short period (usually 72 °C for 15 seconds). However, the time/temperature combination may vary depending on the characteristics of the milk and must, in any case, ensure that the final product meets the legal requirements.

During fermentation, milk is kept for a few hours (5–7 h) in a large tank heated to 45 °C (the fermenter) after combining it with two milk enzymes, *Lactobacillus bulgaricus* and *Streptococcus thermophilus*.

To satisfy these two heat demands, obtain a sufficient temperature difference, and guarantee the temperatures required by the users, the CO₂ heat pump was set to produce water at 80 °C and 50 °C from the HT and MT gas coolers, respectively.

Table 2 lists the parameters of the gas coolers used for the simulations.

Table 2. Parameters used for the simulations.

Parameter	High temperature	Medium temperature
Heat load (kW)	127.4	32
Water temperature (°C)	80	50
Milk temperature (°C)	73	45
Milk mass flow rate (L · h ⁻¹)	3.50	3.50

The maximum pressure was set to 100 bar, and the temperature of a typical day in January was considered.

The COP is the ratio between the useful heat and power consumption. Based on Figs. 5 and 6, the power required by the compressor is calculated as follows:

$$P_c = \dot{m}_{\text{CO}_2}(h_{dis} - h_{suc}) \quad (1)$$

The useful rate of heat transferred to water is:

$$\dot{Q} = \dot{m}_{\text{CO}_2}(h_{dis} - h_{outMT}) = \dot{m}_w c_{p,w}(T_{wo} - T_{wi}) \quad (2)$$

Consequently, the COP is given by the ratio of the enthalpy change in the gas cooler (process 2–3 in Fig. 3) to that in the compressor (process 1–2 in Fig. 3):

$$COP = \frac{\dot{Q}}{P_c} = \frac{(h_{dis} - h_{outMT})}{(h_{dis} - h_{suc})} \quad (3)$$

In these equations, \dot{m}_{CO_2} , h , \dot{m}_w , and $c_{p,w}$ denote the mass flow rate of CO₂, enthalpy of the refrigerant, water mass flow rate, and specific heat capacity, respectively. T_{wi} and T_{wo} are the water inlet and outlet temperatures, respectively.

Equation 3 indicates that the energy efficiency of the heat pump may be increased by increasing the heat rejected or reducing the compressor power, or both. The enthalpy change in the numerator depends on the discharge point of the compressor and working fluid outlet conditions from the MT gas cooler (point 3 in Figs. 2 and 3).

$$h_{dis} = f(p_{dis}, T_{dis}) \quad (4)$$

$$h_{outMT} = f(p_{dis}, T_{outMT}) \quad (5)$$

T_{outMT} is related to the inlet water temperature and the efficiency of the heat exchanger.

After the end-user demands are defined, the useful thermal capacity is a design parameter of the heat pump, with little scope for modification. However, it is convenient to use the denominator of the COP to reduce the increase in the enthalpy of the compressor.

$$h_{suc} = f(p_{ev}, T_{suc}) \quad (6)$$

$$h_{dis} = f(h_{suc}, \eta_{is}) \quad (7)$$

Transcritical CO₂ heat pumps cannot be made competitive by simply choosing a high isentropic efficiency compressor. Moreover, as manufacturing technology has reached sufficient maturity level, little improvement is expected. Acting on evaporation conditions is the best option from a thermodynamic perspective; therefore, all studies that aim to improve this innovative technology

focus on ejectors or double compressions. As mentioned, these solutions are fairly expensive compared to the simple cycle because of equipment costs and management, especially when a very high thermal capacity is required, such as in the industrial field. In this study, the effect of using warm water to increase the evaporation temperature and, consequently, the evaporation pressure, directly reflects on the denominator of the fraction.

3. Results and discussion

Two different simulations were conducted to determine how the heat recovery system improved system performance. First, the heat pump was run from 8 a.m. to 6 p.m. on a typical January day. This ensured that the air temperature was the least favorable considering the location chosen (central Italy). Pasteurization and fermentation are the only processes that are fed by the heat of the gas coolers during this period. Fig. 7 shows the COP during the day, which follows the specific work of the compressor (Fig. 8). Both trends exhibit an accentuated convexity at approximately 2:30 p.m., thereby accounting for the external air temperature used as a boundary condition (Fig. 9). The same trends, but with better performance, can be achieved if higher temperatures are considered, as in June.

The size of the TES must be obtained as a trade-off between the necessity of performing as many discharging cycles as possible in a working day and the physical limitations of the system's inertia. If the tank is too large, its charge and discharge will be too long and render the daily COP increment irrelevant. In contrast, if the tank is too small, the heat pump will be unable to physically follow the hydronic circuit because of the continual switching between the air and water evaporator. To define a tentative size for the TES, an operating time of 1 h was chosen for the charge and discharge cycles, and the recoverable heat rate was evaluated. According to this, the amount of heat that could be stored in the TES was 167.4 kWh. Considering a change of 50 K in the water temperature, the corresponding water volume is 2800 L. Considering the commercially available water tank sizes and the overall size of the hydronic circuit, 3000 L is a suitable trade-off between the costs and benefits on the discharging time. However, to assess the impact of the TES size on the performance of the system, a parametric analysis was conducted, considering changes in the tank volume in the range of 3,000 – 3,800 L. Fig. 10 shows the discharging COP during the first hours of the day, in which the trends are not influenced by the volume as the maximum COP is always approximately 4. Finally, several rounds of simulations were performed to determine the results of using a heat recovery system. The 3,000-L water tank can be charged and then discharged completely in less than an hour by rejecting heat to CO₂ through a water evaporator. Considering the same daily working time, a series of charging and discharging phases were performed sequentially. The total COP of the system is presented in Fig. 11. Although the performance of the charging phase is the same as that of the base cycle, the COP of the discharging step is clearly different. This trend is consistent with that described previously: the progressive cooling of water reduces the evaporation temperature and pressure; simultaneously, the compressor work increases, leading to lower COPs. The discharge stops when a threshold temperature is reached in the tank and a new charging cycle is initiated.

The overall COPs were calculated as a weighted average over time, and the results, compared with those of the basic cycle, are listed in Table 3.

Table 3. Percentage deviations of the average daily COPs between the basic heat pump configuration and that with TES

$COP_{\text{base cycle}}$	$COP_{\text{heat recovery system}}$	Difference	Difference (%)
2.9075	3.0423	0.1347	+4.43

Note: coefficient of performance (COP); thermal energy storage (TES).

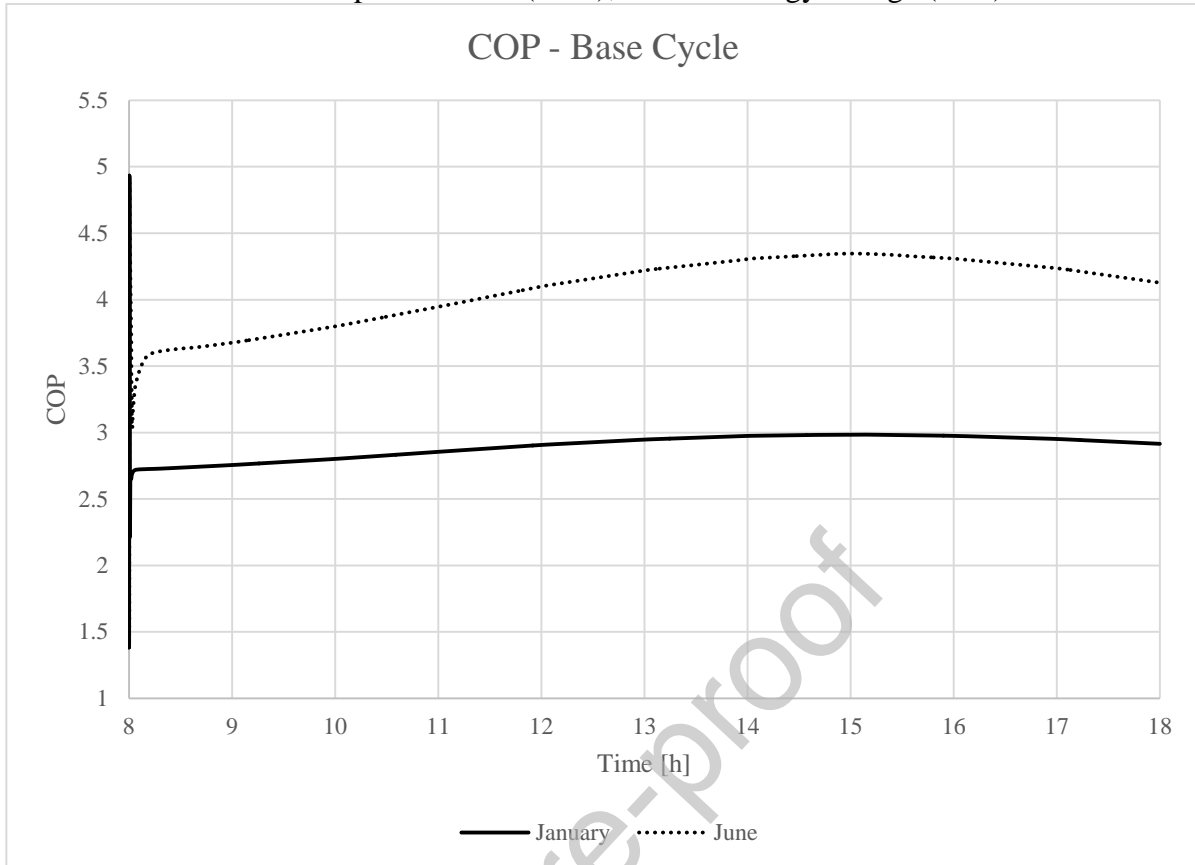


Fig.7. COP considering a basic cycle in January and June

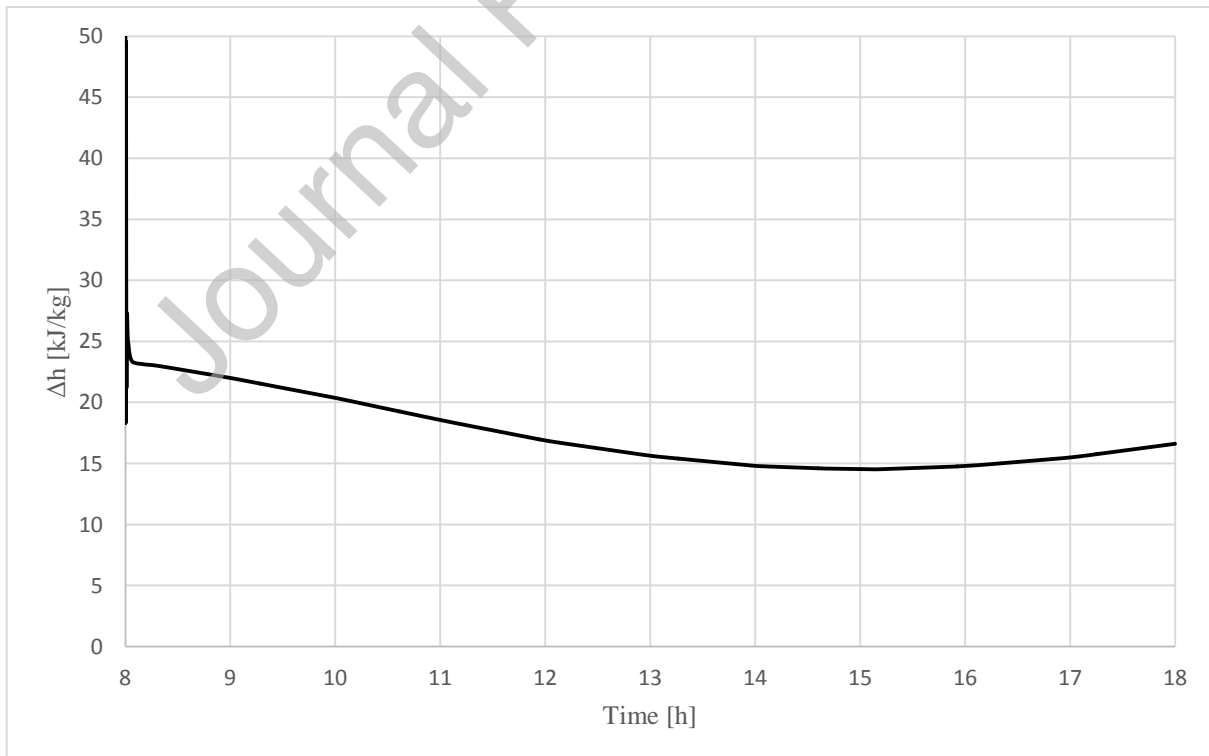


Fig. 8. Specific work of the compressor

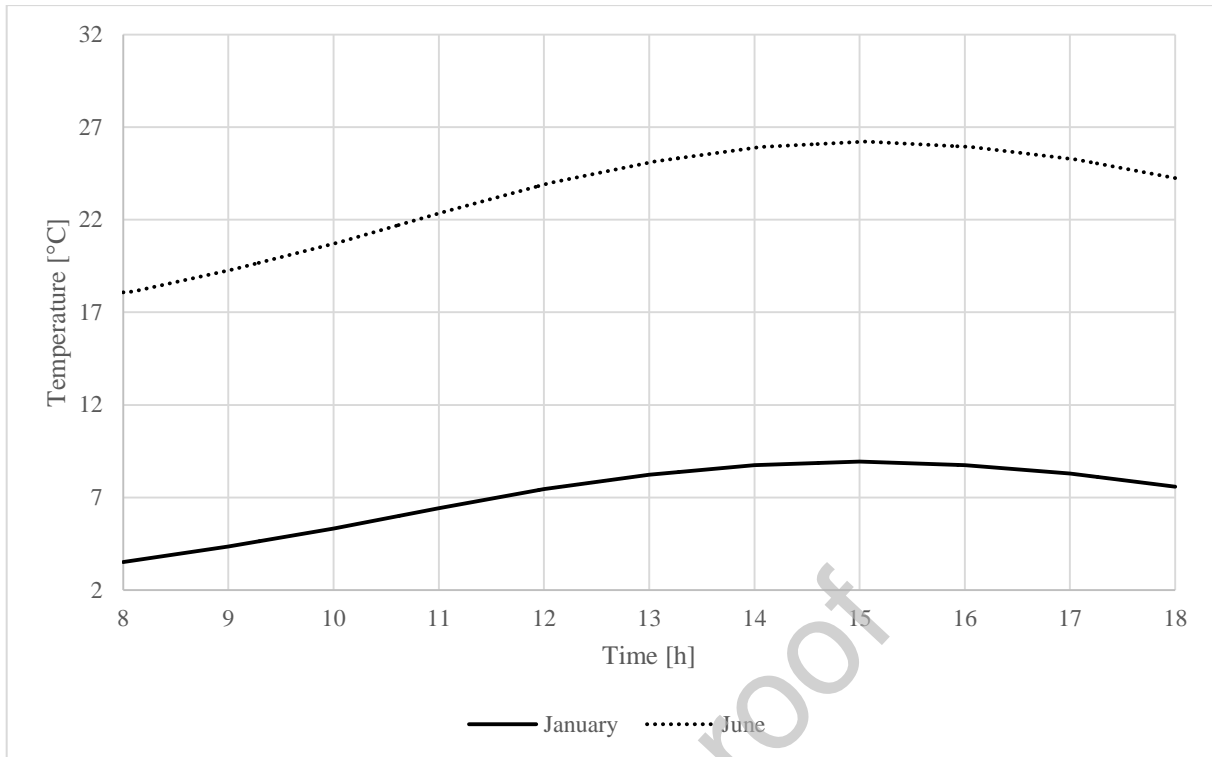


Fig. 9. Temperature of the external air temperature

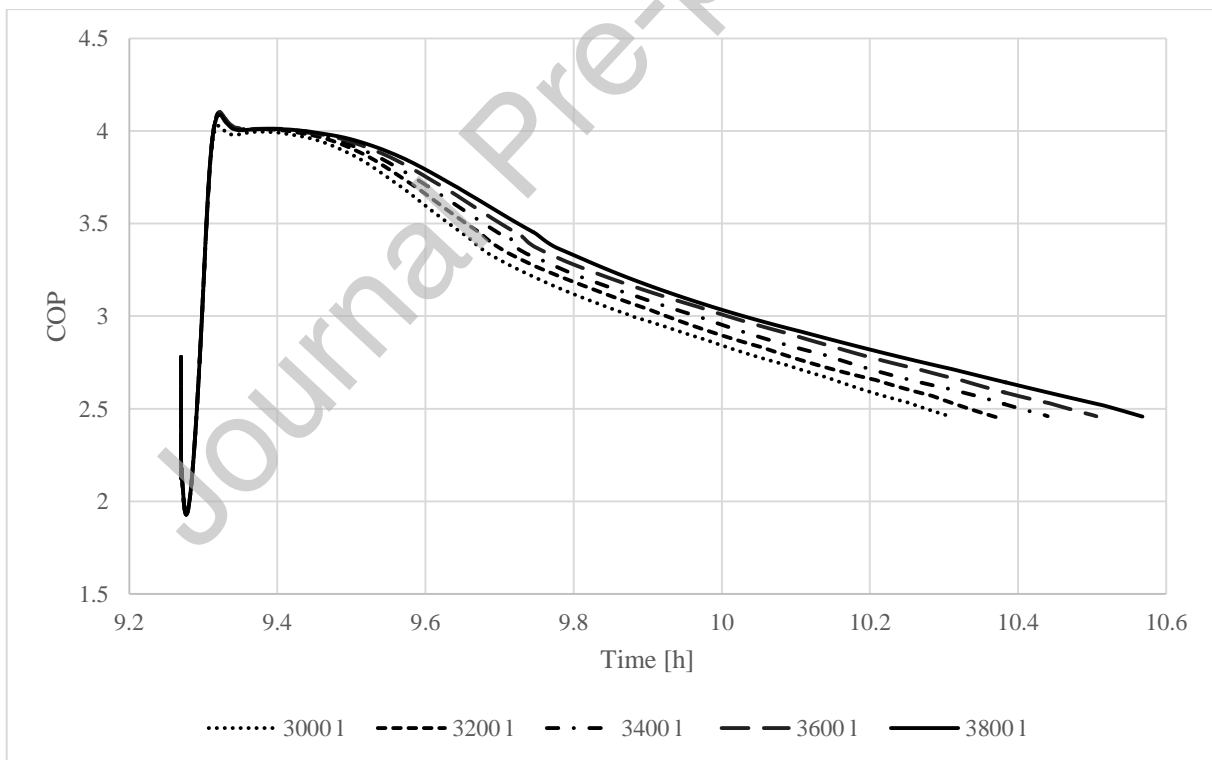


Fig. 10. Discharging COP with changing tank volume

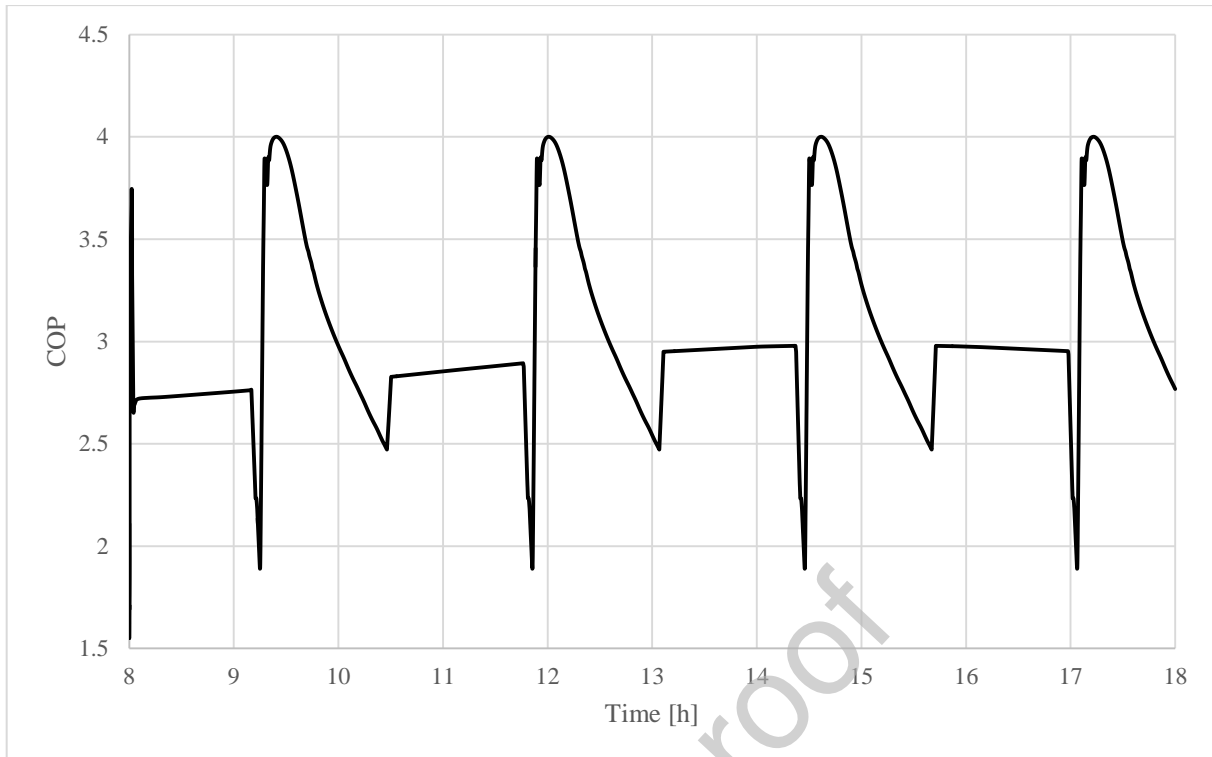


Fig.11. Overall COP of the heat recovery system

4. Conclusions

As a refrigerant, CO₂ can contribute to a less-polluted environment and safer workspaces. Its thermophysical and thermodynamic properties make it suitable for heat pumps, which are major candidates for decarbonizing the heating sector. Transcritical CO₂ heat pumps have been widely discussed in the civil and residential sectors; however, more research is required for their industrial application. Considering a dairy plant as a case study, we focused on the possibilities of using such energy conversion systems in an innovative, simple, and cheap configuration compared with those discussed in the literature. The combination of a water tank for heat storage and a transcritical CO₂ heat pump with two different evaporators can increase the COP through heat recovery cycles.

The heat recovery system showed promising results, yielding an increase of 4.43% in the COP of the base cycle. Its performance can be further improved by increasing the number of discharging phases during the day by improvements in the water tank itself and accelerating the discharging time.

Nomenclature

CO ₂	Carbon dioxide
HFCs	Hydrofluorocarbons
COP	Coefficient of performance
TES	Thermal energy storage
CFCs	Chlorofluorocarbons
HCFCs	Hydrochlorofluorocarbons
ODP	Ozone depletion potential
GWP	Global warming potential
CIP	Cleaning in place
IHX	Internal heat exchanger

HT GC High-temperature gas cooler
 MT GC Medium-temperature gas cooler

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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